Tris(2-hydroxyethyl) isocyanurate 839-90-7 | DTXSID4026266

839-90-7	DTXSID4026266	

Model Performance

Model	Data

Weighted KNN model

5-fold CV (7	5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.84	0.55	0.85	0.53	0.83	0.64	

Model Results

Predicted value: 1.61

Global applicability domain: Outside

Local applicability domain index: 2.42e-01

Confidence level: 7.79e-01

Nearest Neighbors from the Training Set

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Tris(2-hydroxyethyl) isocyanurate

Measured: 1.58 Predicted: 1.61

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Melamine

Measured: 3.80 Predicted: 2.45

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Pentaerythritol

Measured: 1.26 **Predicted:** 1.25

Image not found

Triethanolamine Measured: 3.89 Predicted: 2.97

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Triisopropanolamine Measured: 5.75e-01 Predicted: 7.42e-01